

SAFETY DATA SHEET

1. Identification

Product identifier	cis-3-HEXENYL ALPHA METHYL BUTYRATE FCC	
Other means of identification		
BRI Product Code	103	
CAS number	53398-85-9	
FEMA number	3497	
Synonyms	(* Alt. CAS #) CAS: 10094-41-4; 3-Hexenyl 2-methylbutanoate * Butanoic acid, 2-methyl-, (3Z)-3-hexenyl ester * cis-3-Hexenyl 2-methyl butyrate * cis-3-Hexenyl 2-methylbutanoate * cis-3-Hexenyl 2-methylbutyrate * FEMA CAS: 10094-41-4 * z-3-Hexenyl-2-methylbutyrate	
Recommended use	flavors and fragrances For Manufacturing Use Only	
Recommended restrictions	Not for use in Tobacco or Nicotine delivery device applications and/or products.	
Manufacturer/Importer/Supplier/Distributor information		
Manufacturer		
Company name	Bedoukian Research	
Address	6 Commerce Drive Danbury, CT 06810 United States	
Telephone	1-203-830-4000	
Website	www.bedoukian.com	
E-mail	customerservice@bedoukian.com	
Contact person	Joseph Bania	
Emergency phone number	Chemtrec (North America)	1-800-424-9300
	Chemtrec (International)	1-703-527-3887

2. Hazard(s) identification

Physical hazards	Flammable liquids	Category 4
Health hazards	Not classified.	
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	
Label elements		
Hazard symbol	None.	
Signal word	Warning	
Hazard statement	Combustible liquid.	
Precautionary statement		
Prevention	Keep away from flames and hot surfaces-No smoking. Wear protective gloves/eye protection/face protection.	
Response	In case of fire: Use appropriate media to extinguish.	
Storage	Store in a well-ventilated place. Keep cool.	
Disposal	Dispose of contents/container in accordance with relevant area regulations.	
Hazard(s) not otherwise classified (HNOC)	None known.	
Supplemental information	100% of the mixture consists of component(s) of unknown acute inhalation toxicity. 100% of the mixture consists of component(s) of unknown acute hazards to the aquatic environment. 100% of the mixture consists of component(s) of unknown long-term hazards to the aquatic environment. Contains synthetic alpha tocopherol. May produce an allergic reaction.	

3. Composition/information on ingredients

Substances

Chemical name	Common name and synonyms	CAS number	%
cis-3-HEXENYL ALPHA METHYL BUTYRATE FCC	(* Alt. CAS #) CAS: 10094-41-4; 3-Hexenyl 2-methylbutanoate Butanoic acid, 2-methyl-, (3Z)-3-hexenyl ester cis-3-Hexenyl 2-methyl butyrate cis-3-Hexenyl 2-methylbutanoate cis-3-Hexenyl 2-methylbutyrate FEMA CAS: 10094-41-4 z-3-Hexenyl-2-methylbutyrate	53398-85-9	100

Stabilizers

Chemical name	Common name and synonyms	CAS number	%
synthetic alpha tocopherol		10191-41-0	0.1

*Designates that a specific chemical identity and/or percentage of composition has been withheld as a trade secret.

Composition comments Occupational Exposure Limits for stabilizers are listed in Section 8.

4. First-aid measures

Inhalation	Move to fresh air. Call a physician if symptoms develop or persist.
Skin contact	Wash off with soap and water. Get medical attention if irritation develops and persists.
Eye contact	Rinse with water. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. Get medical attention if symptoms occur.
Most important symptoms/effects, acute and delayed	Direct contact with eyes may cause temporary irritation.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically.
General information	Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves.

5. Fire-fighting measures

Suitable extinguishing media	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO ₂).
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
Specific hazards arising from the chemical	The product is combustible, and heating may generate vapors which may form explosive vapor/air mixtures. During fire, gases hazardous to health may be formed.
Special protective equipment and precautions for firefighters	Self-contained breathing apparatus and full protective clothing must be worn in case of fire.
Fire fighting equipment/instructions	In case of fire and/or explosion do not breathe fumes. Move containers from fire area if you can do so without risk.
Specific methods	Use standard firefighting procedures and consider the hazards of other involved materials.
General fire hazards	Combustible liquid.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. Keep people away from and upwind of spill/leak. Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Wear appropriate protective equipment and clothing during clean-up. Ensure adequate ventilation. Local authorities should be advised if significant spillages cannot be contained. For personal protection, see section 8 of the SDS.
Methods and materials for containment and cleaning up	Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Keep combustibles (wood, paper, oil, etc.) away from spilled material. Large Spills: Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible. Use a non-combustible material like vermiculite, sand or earth to soak up the product and place into a container for later disposal. Following product recovery, flush area with water. Small Spills: Absorb with earth, sand or other non-combustible material and transfer to containers for later disposal. Clean surface thoroughly to remove residual contamination. Never return spills to original containers for re-use. For waste disposal, see section 13 of the SDS.
Environmental precautions	Avoid discharge into drains, water courses or onto the ground.

7. Handling and storage

Precautions for safe handling	Keep away from open flames, hot surfaces and sources of ignition. When using do not smoke. Provide adequate ventilation. Wear appropriate personal protective equipment. Observe good industrial hygiene practices.
Conditions for safe storage, including any incompatibilities	Keep away from heat, sparks and open flame. Store in a cool, dry place out of direct sunlight. Store in original tightly closed container. Store in a well-ventilated place. Keep in an area equipped with sprinklers. Store away from incompatible materials (see Section 10 of the SDS). Recommended Packaging: Glass, Plastic, Aluminum or Phenolic Lined Steel. Store tightly sealed under inert gas in a cool, well-ventilated area.

8. Exposure controls/personal protection

Occupational exposure limits	This substance has no PEL, TLV, or other recommended exposure limit.
Biological limit values	No biological exposure limits noted for the ingredient(s).
Appropriate engineering controls	Good general ventilation (typically 10 air changes per hour) should be used. Ventilation rates should be matched to conditions. If applicable, use process enclosures, local exhaust ventilation, or other engineering controls to maintain airborne levels below recommended exposure limits. If exposure limits have not been established, maintain airborne levels to an acceptable level.
Individual protection measures, such as personal protective equipment	
Eye/face protection	Wear safety glasses with side shields (or goggles).
Skin protection	
Hand protection	Wear appropriate chemical resistant gloves.
Other	Wear suitable protective clothing.
Respiratory protection	If engineering controls do not maintain airborne concentrations below recommended exposure limits (where applicable) or to an acceptable level (in countries where exposure limits have not been established), an approved respirator must be worn.
Thermal hazards	Wear appropriate thermal protective clothing, when necessary.
General hygiene considerations	When using do not smoke. Always observe good personal hygiene measures, such as washing after handling the material and before eating, drinking, and/or smoking. Routinely wash work clothing and protective equipment to remove contaminants.

9. Physical and chemical properties

Appearance	
Physical state	Liquid.
Color	colorless to pale yellow
Odor	a 'natural' fruity odor of green apples.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	Not available.
Initial boiling point and boiling range	435.51 °F (224.17 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Flash point	180 °F (82 °C) Closed Cup
Evaporation rate	Not available.
Flammability (solid, gas)	Not applicable.
Upper/lower flammability or explosive limits	
Flammability limit - lower (%)	Not available.
Flammability limit - upper (%)	Not available.
Explosive limit - lower (%)	Not available.
Explosive limit - upper (%)	Not available.
Vapor pressure	0.07 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	6.4 Relative to air; air = 1
Relative density	Not available.

Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	4.01 US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Auto-ignition temperature	Not available.
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Density	0.876 - 0.880 g/cm3
Explosive properties	Not explosive.
Flammability class	Combustible IIIA estimated
Molecular formula	C11H20O2
Molecular weight	184.28
Oxidizing properties	Not oxidizing.
Specific gravity	0.876 - 0.88 at 25°C

10. Stability and reactivity

Reactivity	The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability	Material is stable under normal conditions.
Possibility of hazardous reactions	Hazardous polymerization does not occur.
Conditions to avoid	Avoid heat, sparks, open flames and other ignition sources. Avoid temperatures exceeding the flash point. Contact with incompatible materials.
Incompatible materials	Strong oxidizing agents.
Hazardous decomposition products	No hazardous decomposition products are known.

11. Toxicological information

Information on likely routes of exposure

Inhalation	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
Skin contact	May cause an allergic skin reaction.
Eye contact	Direct contact with eyes may cause temporary irritation.
Ingestion	Expected to be a low ingestion hazard.

Symptoms related to the physical, chemical and toxicological characteristics Direct contact with eyes may cause temporary irritation.

Information on toxicological effects

Acute toxicity Not known.

Product	Species	Test Results
cis-3-HEXENYL ALPHA METHYL BUTYRATE FCC (CAS 53398-85-9)		
Acute		
Dermal		
<i>Liquid</i>		
LD50	Rabbit	> 5000 mg/kg
Oral		
<i>Liquid</i>		
LD50	Rat	> 5000 mg/kg

* Estimates for product may be based on additional component data not shown.

Skin corrosion/irritation Prolonged skin contact may cause temporary irritation.

Irritation Corrosion - Skin

cis-3-HEXENYL ALPHA METHYL BUTYRATE FCC 10 % Patch test, Vehicle Petrolatum. Result for 3-Hexenyl 2-methylbutanoate CAS 10094-41-4.
Result: No irritation observed.
Species: Human
Organ: Skin
Notes: RIFM

Serious eye damage/eye irritation Direct contact with eyes may cause temporary irritation.

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

Skin sensitization This product is not expected to cause skin sensitization.

Skin sensitization

cis-3-HEXENYL ALPHA METHYL BUTYRATE FCC 10 % Patch test, Vehicle Petrolatum. Result for 3-Hexenyl 2-methylbutanoate CAS 10094-41-4.
Result: Not sensitizing.
Species: Human
Organ: Skin
Notes: RIFM

Germ cell mutagenicity No data available to indicate product or any components present at greater than 0.1% are mutagenic or genotoxic.

Carcinogenicity Not classifiable as to carcinogenicity to humans.

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity This product is not expected to cause reproductive or developmental effects.

Specific target organ toxicity - single exposure Not classified.

Specific target organ toxicity - repeated exposure Not classified.

Aspiration hazard Not an aspiration hazard.

Further information May cause allergic respiratory and skin reactions.

12. Ecological information

Ecotoxicity The product is not classified as environmentally hazardous. However, this does not exclude the possibility that large or frequent spills can have a harmful or damaging effect on the environment.

Persistence and degradability No data is available on the degradability of this product.

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

cis-3-HEXENYL ALPHA METHYL BUTYRATE FCC 4.01, US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

Mobility in soil No data available.

Other adverse effects No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions Collect and reclaim or dispose in sealed containers at licensed waste disposal site. Dispose of contents/container in accordance with local/regional/national/international regulations.

Local disposal regulations Dispose in accordance with all applicable regulations.

Hazardous waste code The waste code should be assigned in discussion between the user, the producer and the waste disposal company.

Waste from residues / unused products Dispose of in accordance with local regulations. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging

Since emptied containers may retain product residue, follow label warnings even after container is emptied. Empty containers should be taken to an approved waste handling site for recycling or disposal.

14. Transport information**DOT**

Not regulated as dangerous goods.

IATA

Not regulated as dangerous goods.

IMDG

Not regulated as dangerous goods.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not established.

15. Regulatory information

US federal regulations This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not regulated.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Hazard categories Immediate Hazard - No
Delayed Hazard - No
Fire Hazard - Yes
Pressure Hazard - No
Reactivity Hazard - No

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical Yes

SARA 313 (TRI reporting)
Not regulated.

Other federal regulations**Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List**

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA) Not regulated.

US state regulations California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins.

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	Yes
Canada	Domestic Substances List (DSL)	Yes
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	Yes
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	Yes

Country(s) or region	Inventory name	On inventory (yes/no)*
Korea	Existing Chemicals List (ECL)	Yes
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	Yes
Taiwan	Taiwan Toxic Chemical Substances (TCS)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)
A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

Issue date	19-May-2015
Revision date	02-April-2021
Version #	02
Disclaimer	Bedoukian Research cannot anticipate all conditions under which this information and its product, or the products of other manufacturers in combination with its product, may be used. It is the user's responsibility to ensure safe conditions for handling, storage and disposal of the product, and to assume liability for loss, injury, damage or expense due to improper use. The information in the sheet was written based on the best knowledge and experience currently available.
Revision information	This document has undergone significant changes and should be reviewed in its entirety.